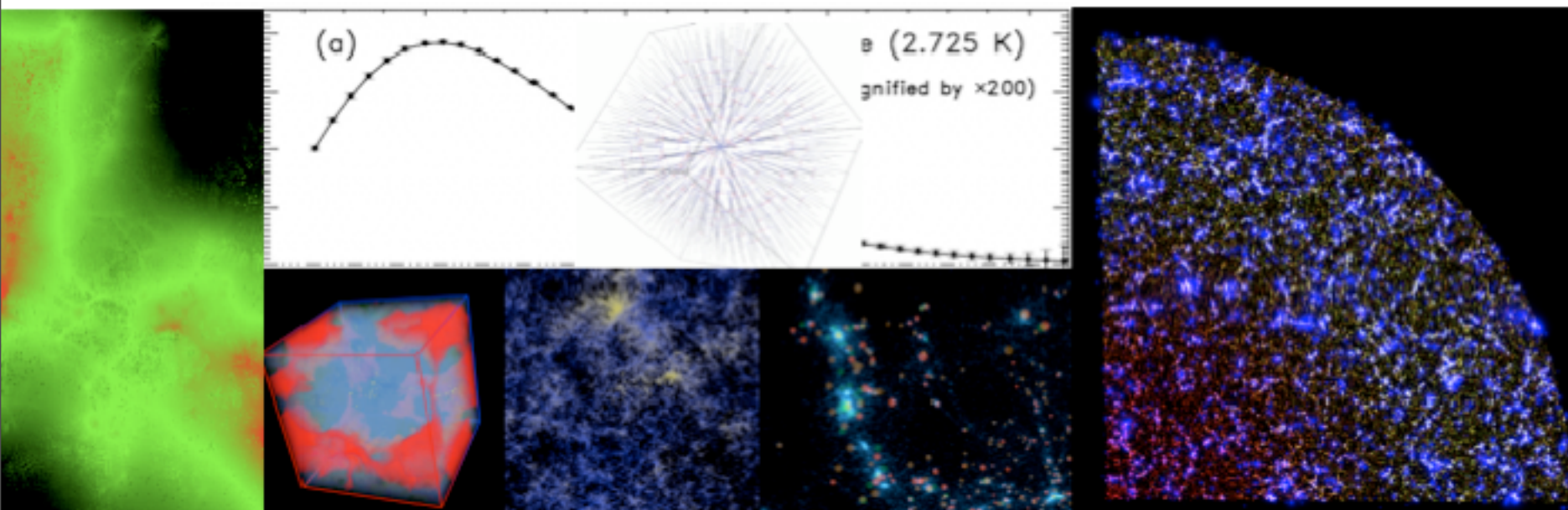


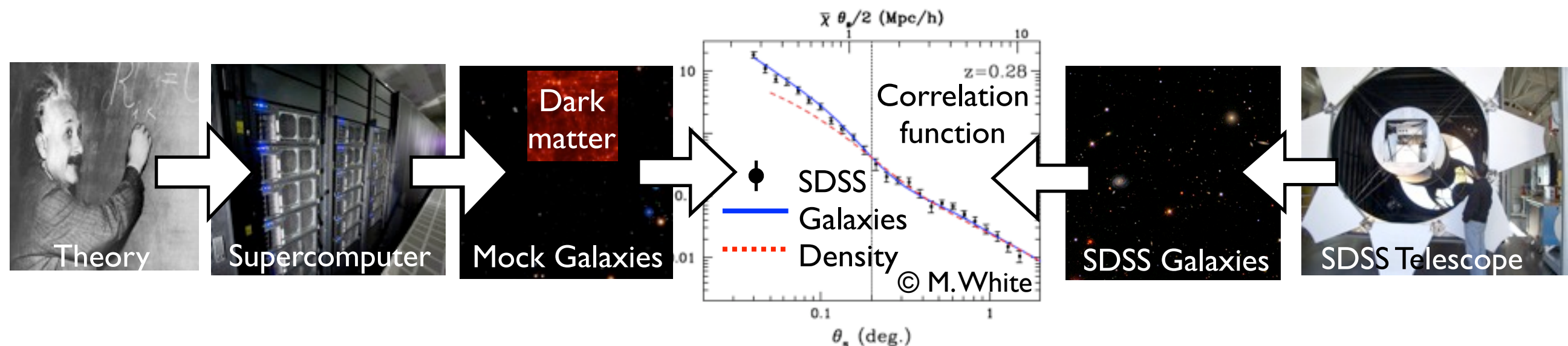
# Large Scale Structure Simulations

Katrin Heitmann

Argonne National Laboratory  
High Energy Physics/  
Mathematics & Computer Science Division



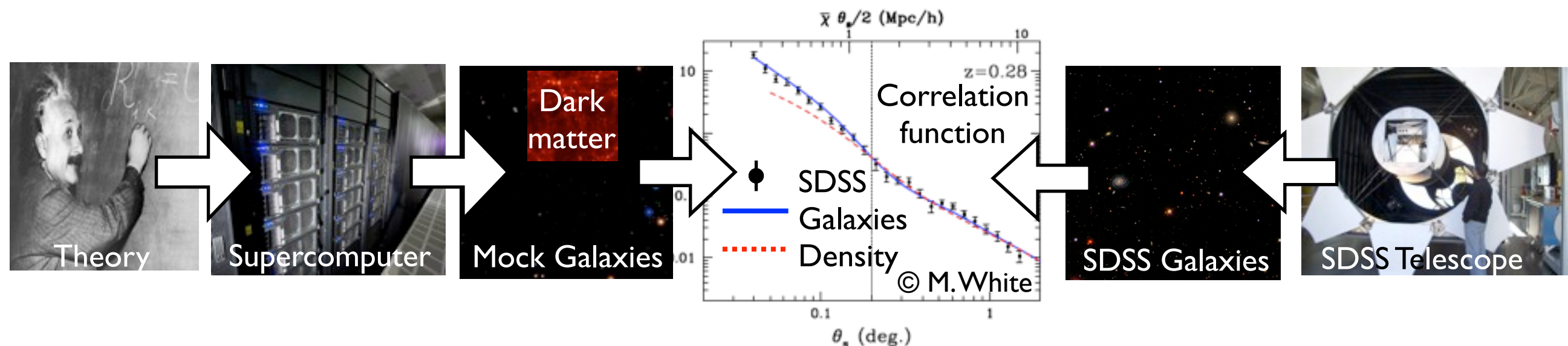
# The Role of N-body Simulations in Cosmology



**All detailed knowledge of structure formation in the nonlinear regime comes from N-body simulations**

- Discovering new physics in the nonlinear regime
- Exploring new cosmological probes
- Analysis of survey results with precision predictions
- Solving cosmological inverse problems
- Basis for generating mock observations
- Estimation of measurement errors

# The Role of N-body Simulations in Cosmology



All detailed knowledge of structure formation in the nonlinear regime comes from N-body simulations

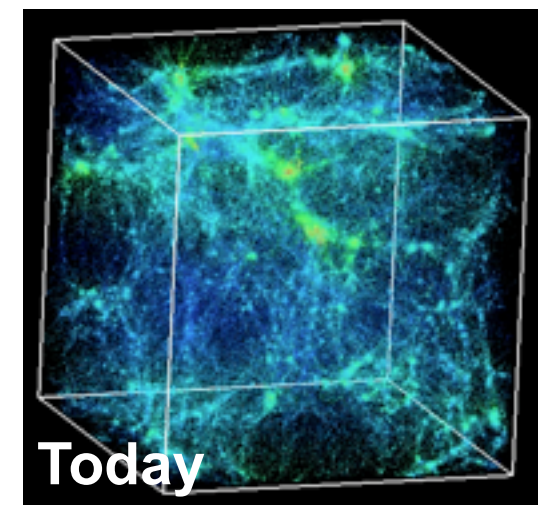
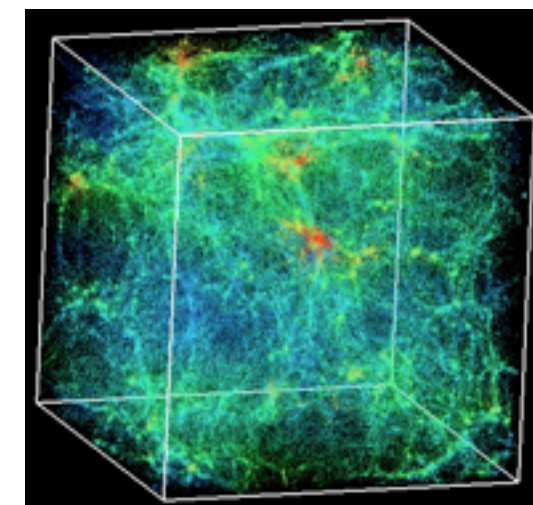
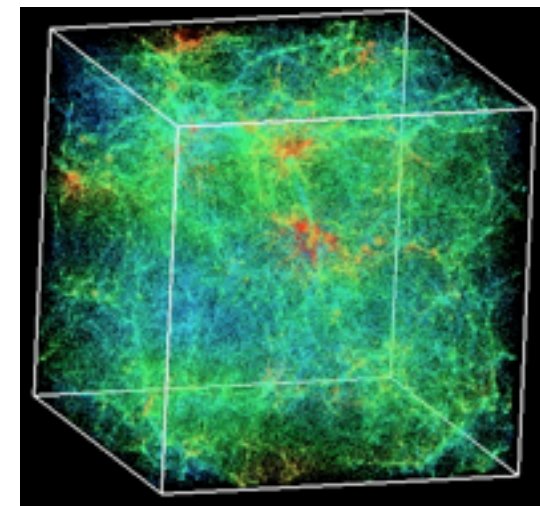
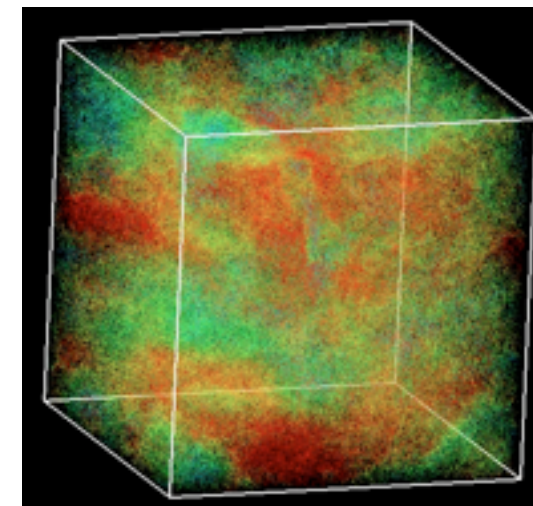
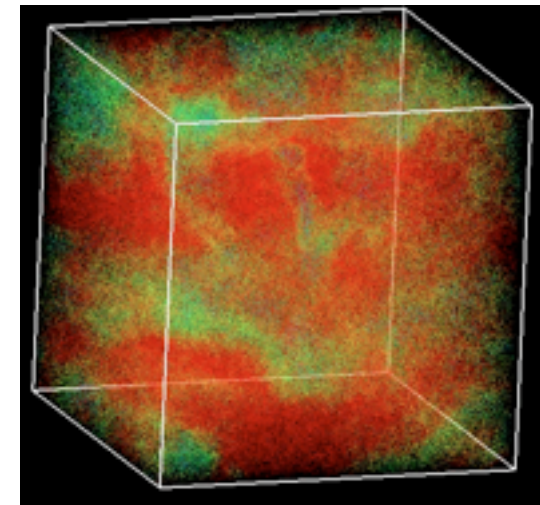
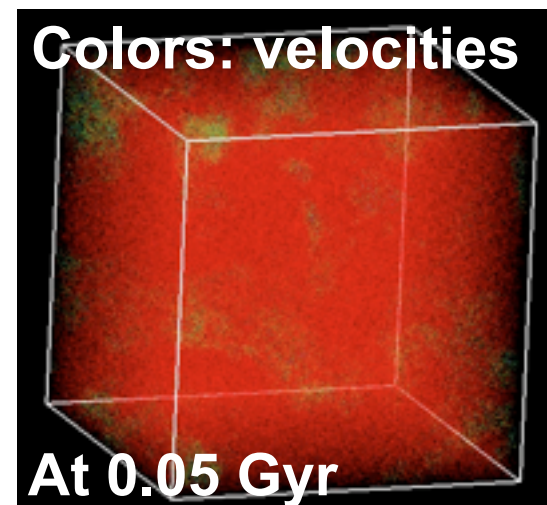
- Discovering new physics in the nonlinear regime
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} Risa's talk



# N-body Simulation Basics

- Follow evolution of dark matter tracer particles in an expanding universe
- Solve Vlasov-Poisson equation
- In principle:  $N^2$  problem ( $N$  = number of particles), in practice, approximate methods based on particle and grid solvers
  - Tree methods: Gadget, HOT, PKDGRAV
  - Adaptive mesh refinement: ART, Enzo, FLASH, **Nyx**, Ramses
  - Hybrid: Gadget-2, **TreePM**, **HACC**



$$\begin{aligned} \frac{\partial f_i}{\partial t} + \dot{\mathbf{x}} \frac{\partial f_i}{\partial \mathbf{x}} - \nabla \phi \frac{\partial f_i}{\partial \mathbf{p}} &= 0, & \mathbf{p} &= a^2 \dot{\mathbf{x}}, \\ \nabla^2 \phi &= 4\pi G a^2 (\rho(\mathbf{x}, t) - \langle \rho_{\text{dm}}(t) \rangle) = 4\pi G a^2 \Omega_{\text{dm}} \delta_{\text{dm}} \rho_{\text{cr}}, \\ \delta_{\text{dm}}(\mathbf{x}, t) &= (\rho_{\text{dm}} - \langle \rho_{\text{dm}} \rangle) / \langle \rho_{\text{dm}} \rangle, \\ \rho_{\text{dm}}(\mathbf{x}, t) &= a^{-3} \sum_i m_i \int d^3 \mathbf{p} f_i(\mathbf{x}, \dot{\mathbf{x}}, t). \end{aligned}$$



# The Virtues of N-body Simulations

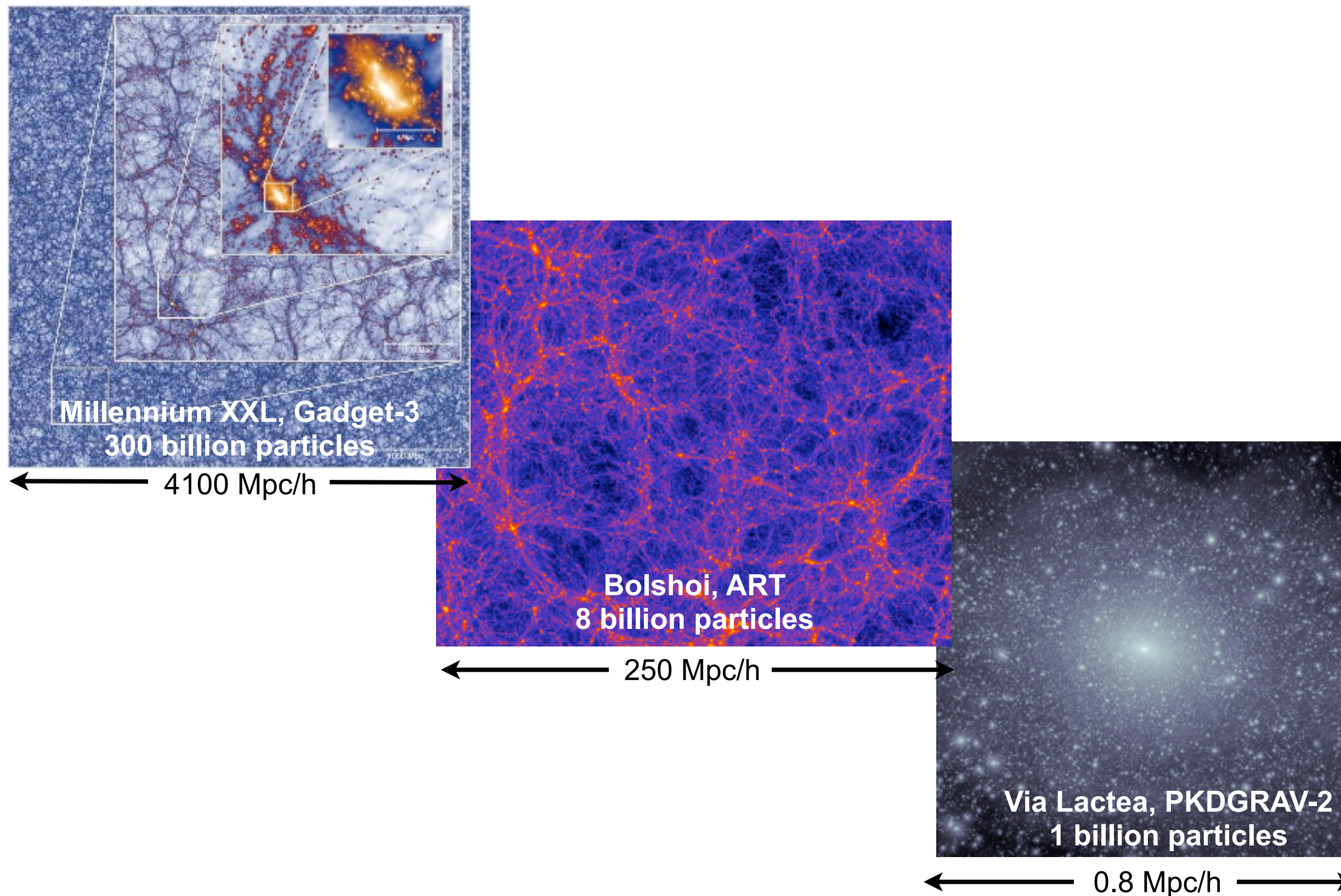
- **Advantages:**

- Capture relevant physics well out into the nonlinear regime
- Cover large dynamic range: from Gigaparsecs down to less than a kiloparsec, therefore allows coverage of survey size volumes
- Underlying physics is well understood
- Several proven numerical paradigms exist, these allow exploration of new high-performance architectures
- No free physics parameters, code parameters can be set to reach sub-percent accuracy
- Simulations can be carried out relatively fast (days to weeks time scale), therefore allow exploration of cosmological parameter space, many realizations can be carried out
- Post-processing via halo occupation distribution models or semi-analytic models allows exploration of additional physics in a straightforward way

- **Disadvantage:**

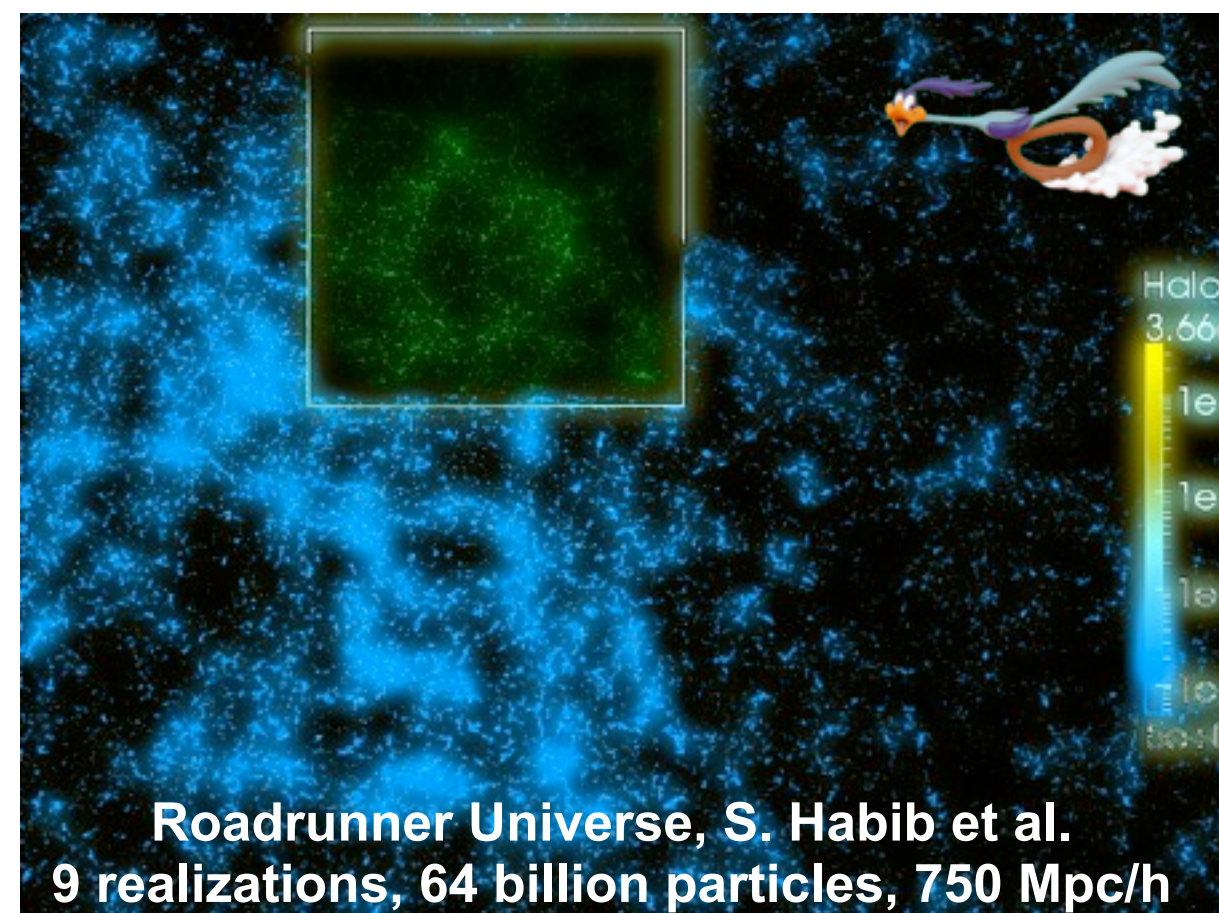
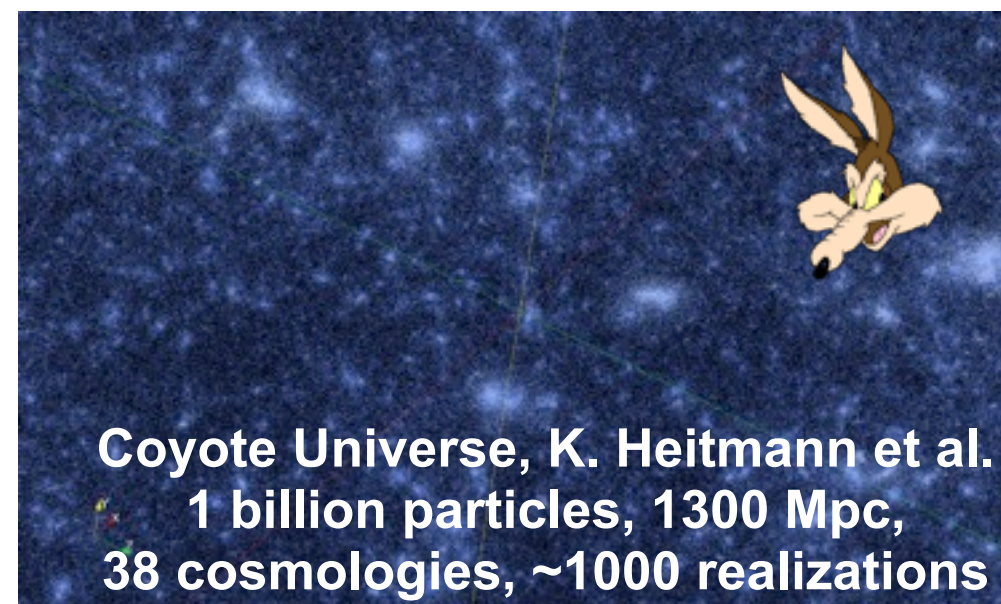
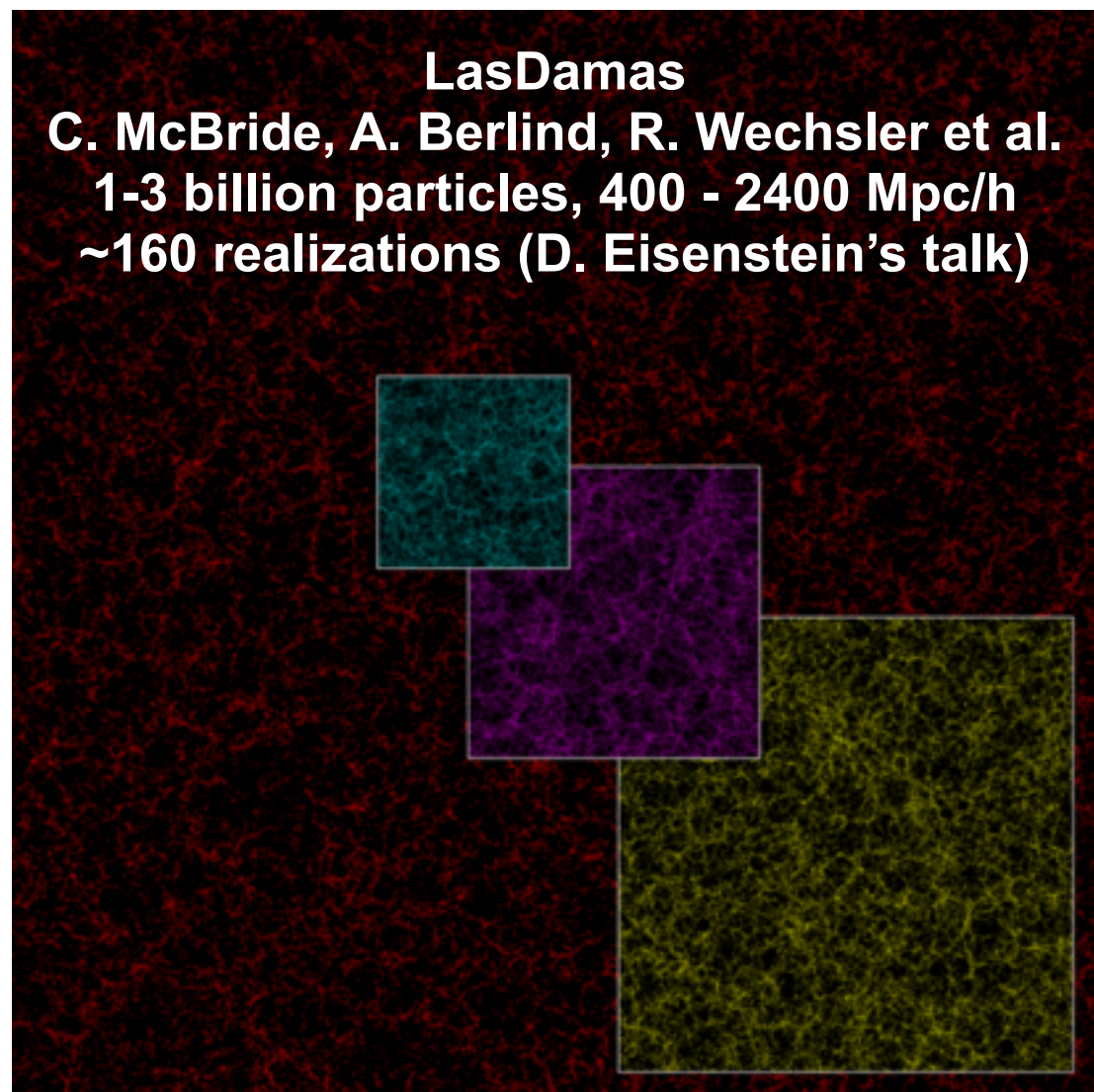
- Miss physics on small scales (gas dynamics, feedback..., see Nick's talk), require phenomenological techniques based on observations (self-calibration)

# Physics Results on All Scales





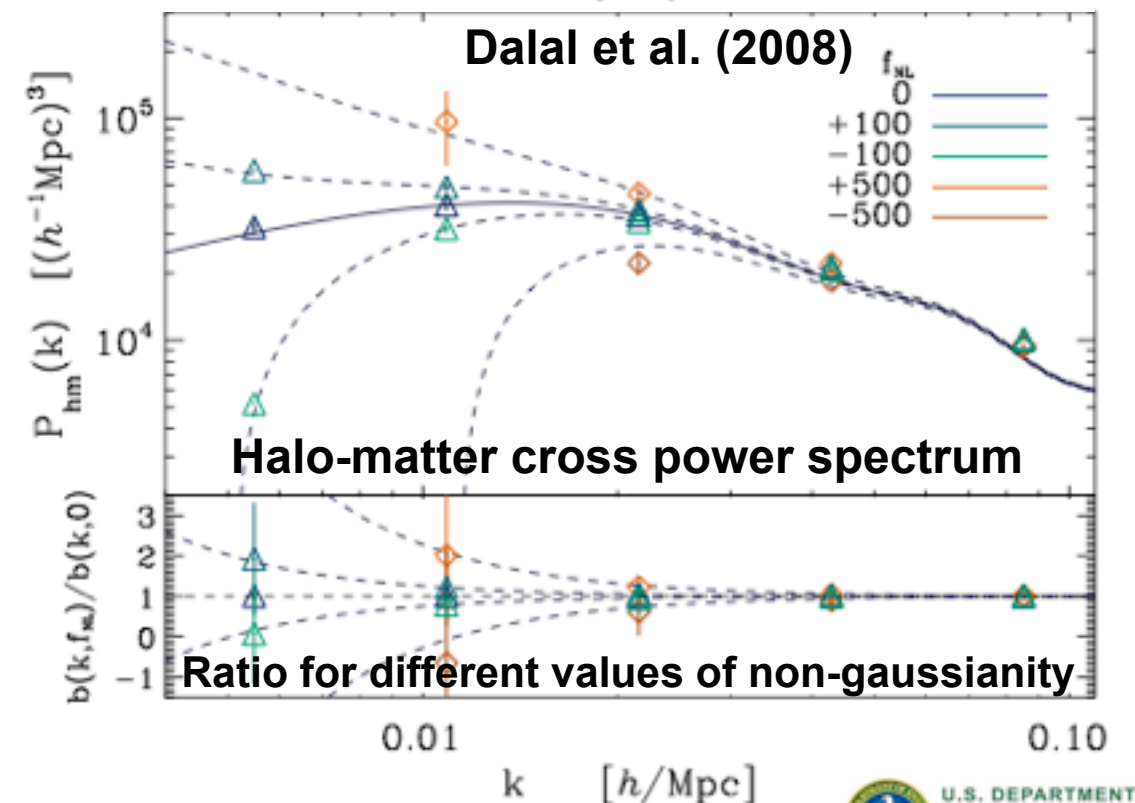
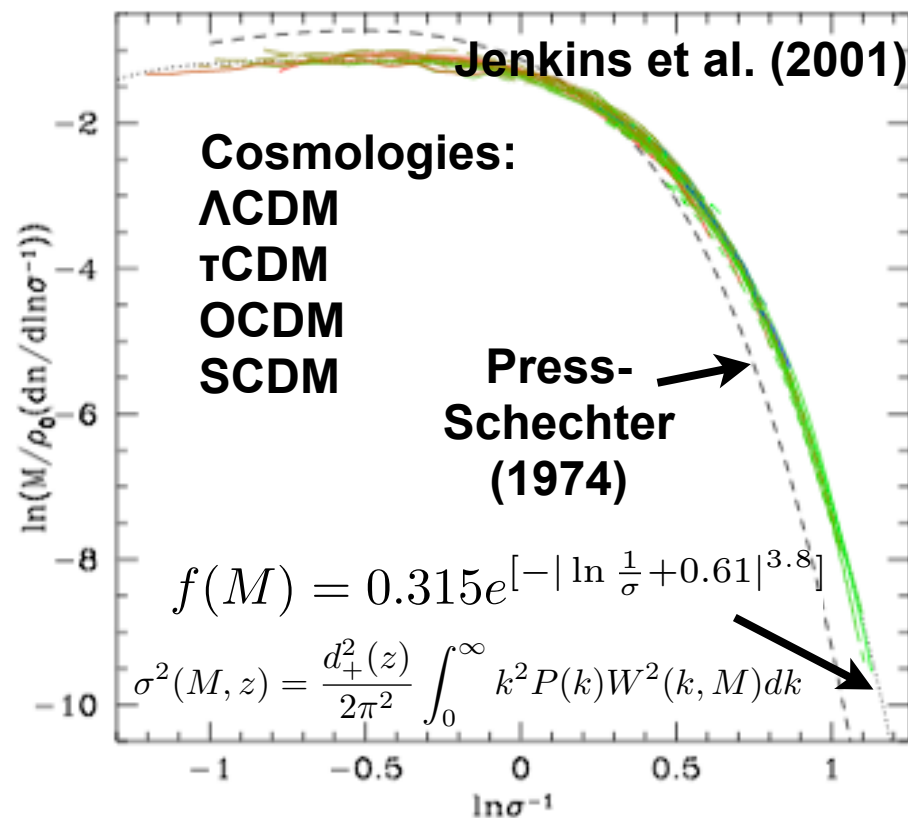
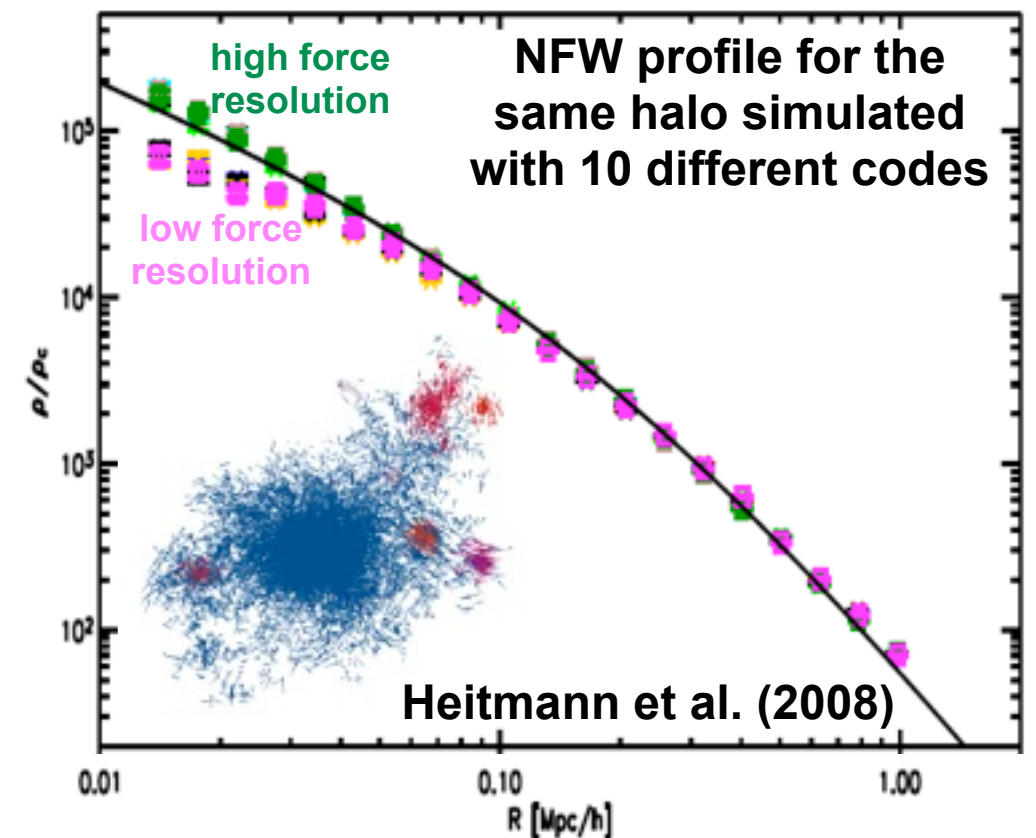
# Surveys Need Statistics!





# Discovering New Physics in the Nonlinear Regime

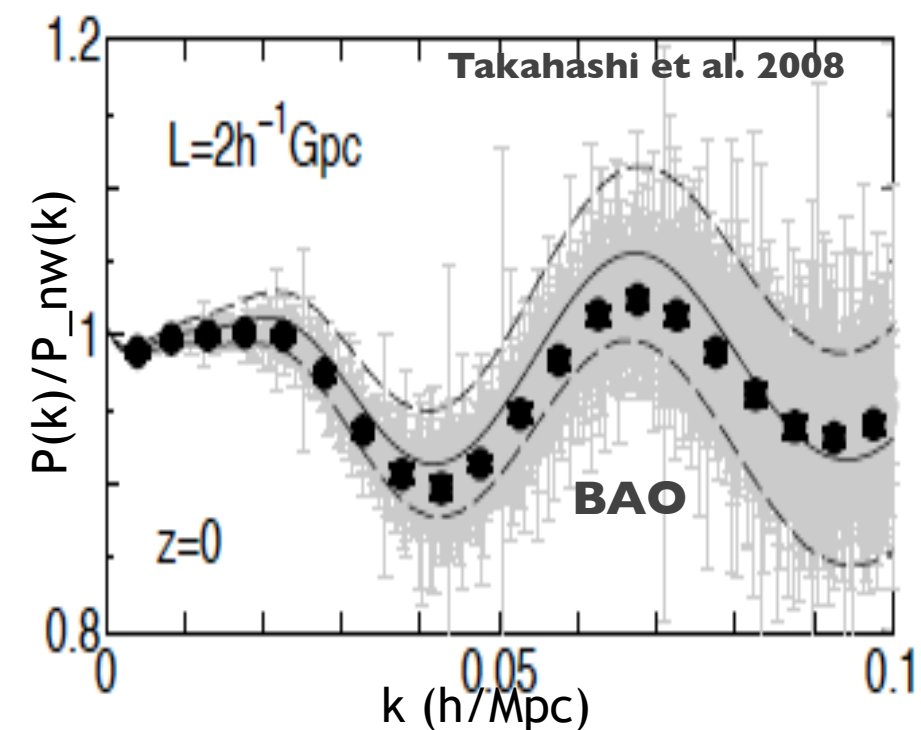
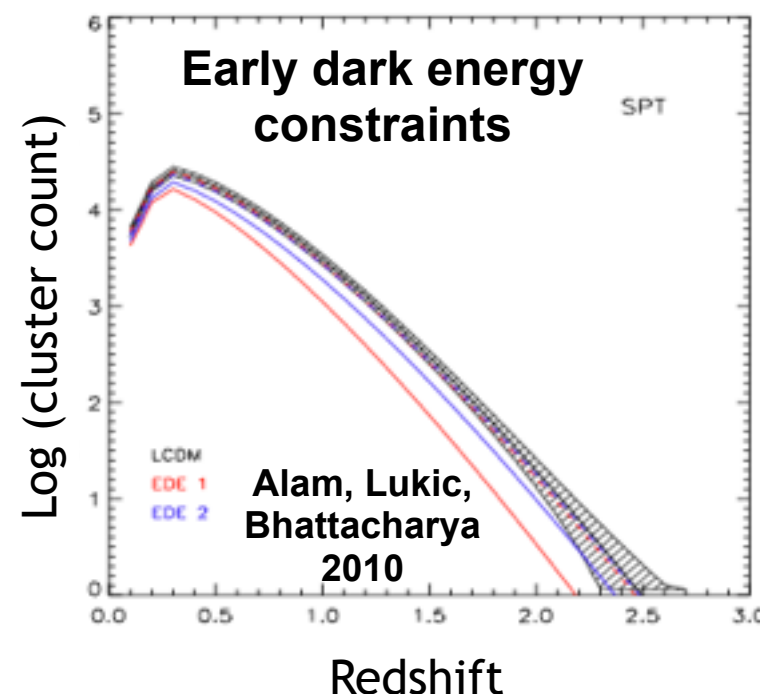
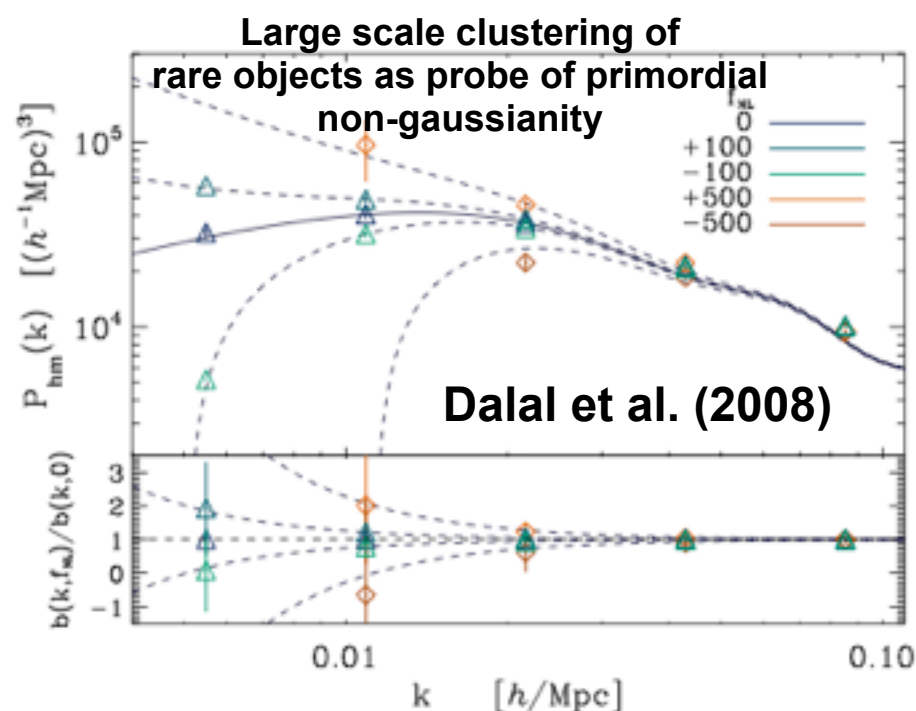
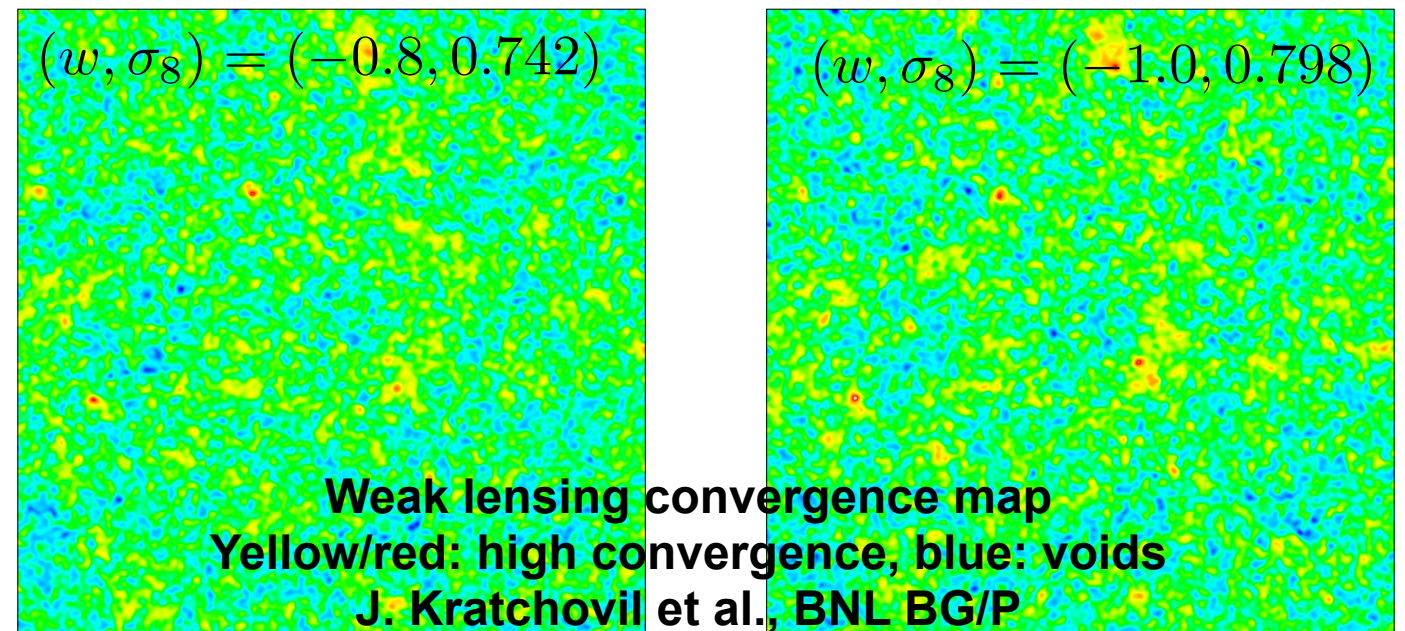
- **Halo profiles:** Navarro, Frenk & White (NFW, 1996, 1997) find that the density profile of a halo as a function of radius has the same shape independent of mass and cosmology
- **Universality of the mass function:** For a particular halo definition (friends-of-friends with a linking length of  $b=0.2$ ) and expressed via the variance of the linear density field  $\sigma^2(z, M)$ , mass function is independent of epoch/cosmology at the 20% level
- **Non-gaussianity/bias:** Non-gaussianity effects clustering of dark matter halos, bias is strongly scale dependent





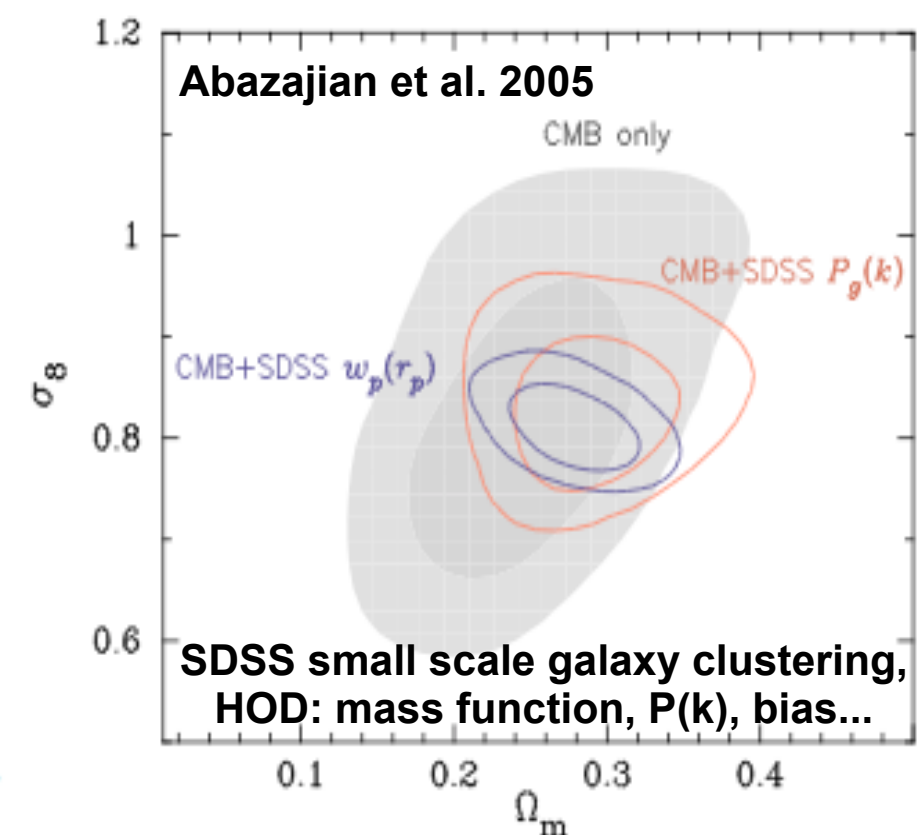
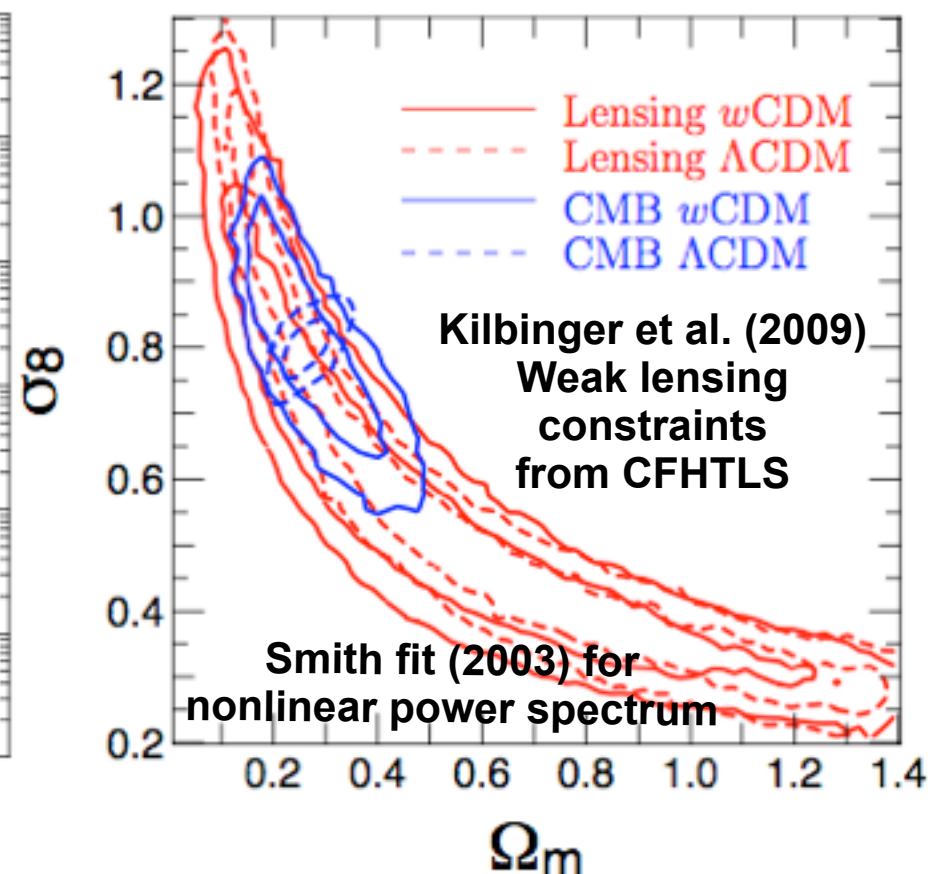
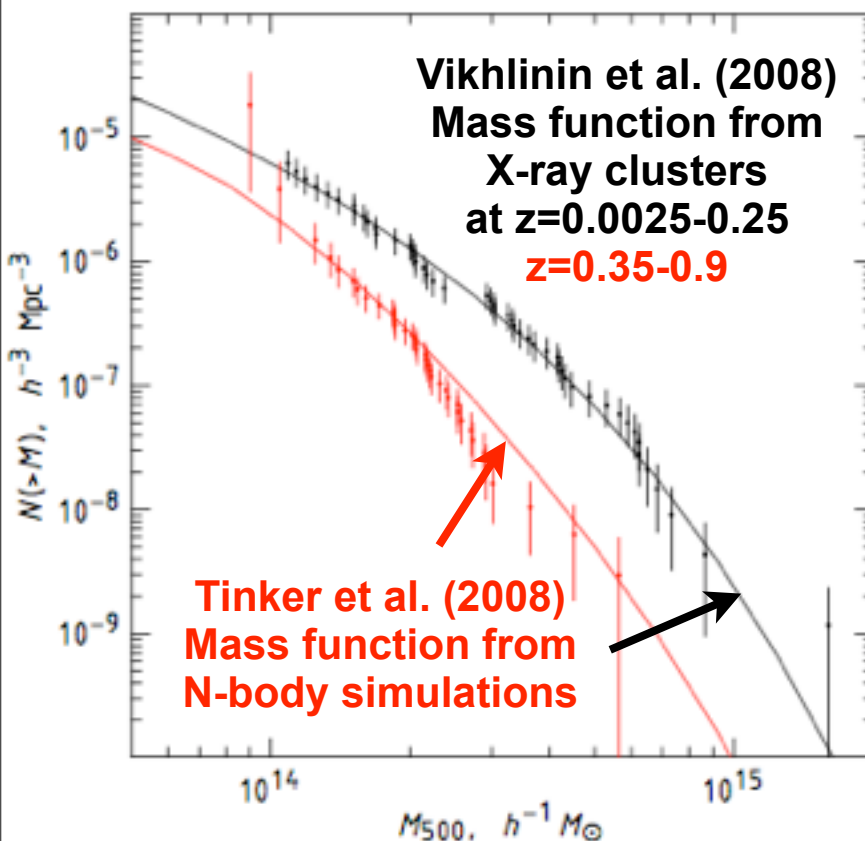
# Exploring New (and Established) Cosmological Probes

- Sensitivity of cosmological probes to new physics (e.g. early dark energy, modified gravity)
- Estimate of the strength of expected signal over noise
- New cosmological probes



# Analysis of Survey Results: Three Examples

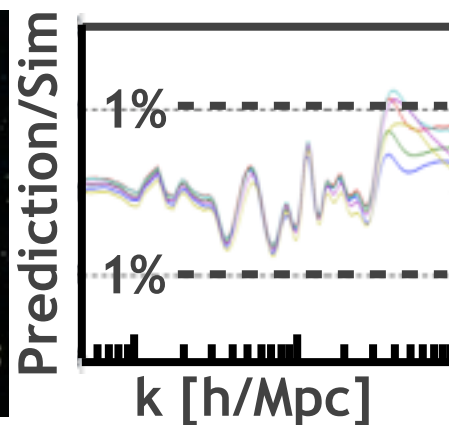
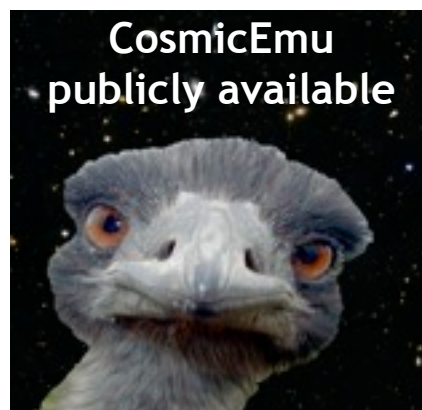
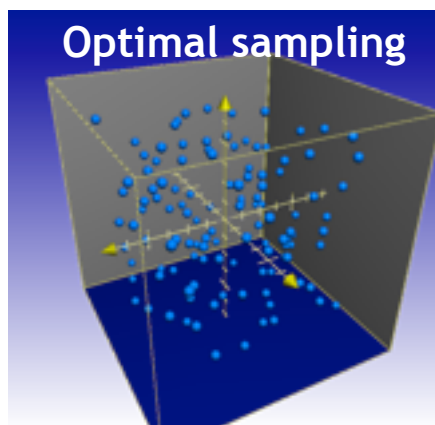
- **Cluster Cosmology:** Cosmological constraints from Chandra X-ray cluster observations, mass function matched to Tinker et al. 2008 fit from N-body simulations
- **Weak lensing:** Cosmological constraints from Canada-France-Hawaii-Telescope Legacy Survey (CFHTLS), Markov Chain Monte Carlo calculations based on Smith (Halo) fit for nonlinear power spectrum (calibrated with N-body simulations)
- **Small scale galaxy clustering:** Cosmological constraints from Sloan Digital Sky Survey, modeling based on Halo Occupancy Distribution (HOD), includes calibration of mass function, power spectrum, bias from N-body simulations



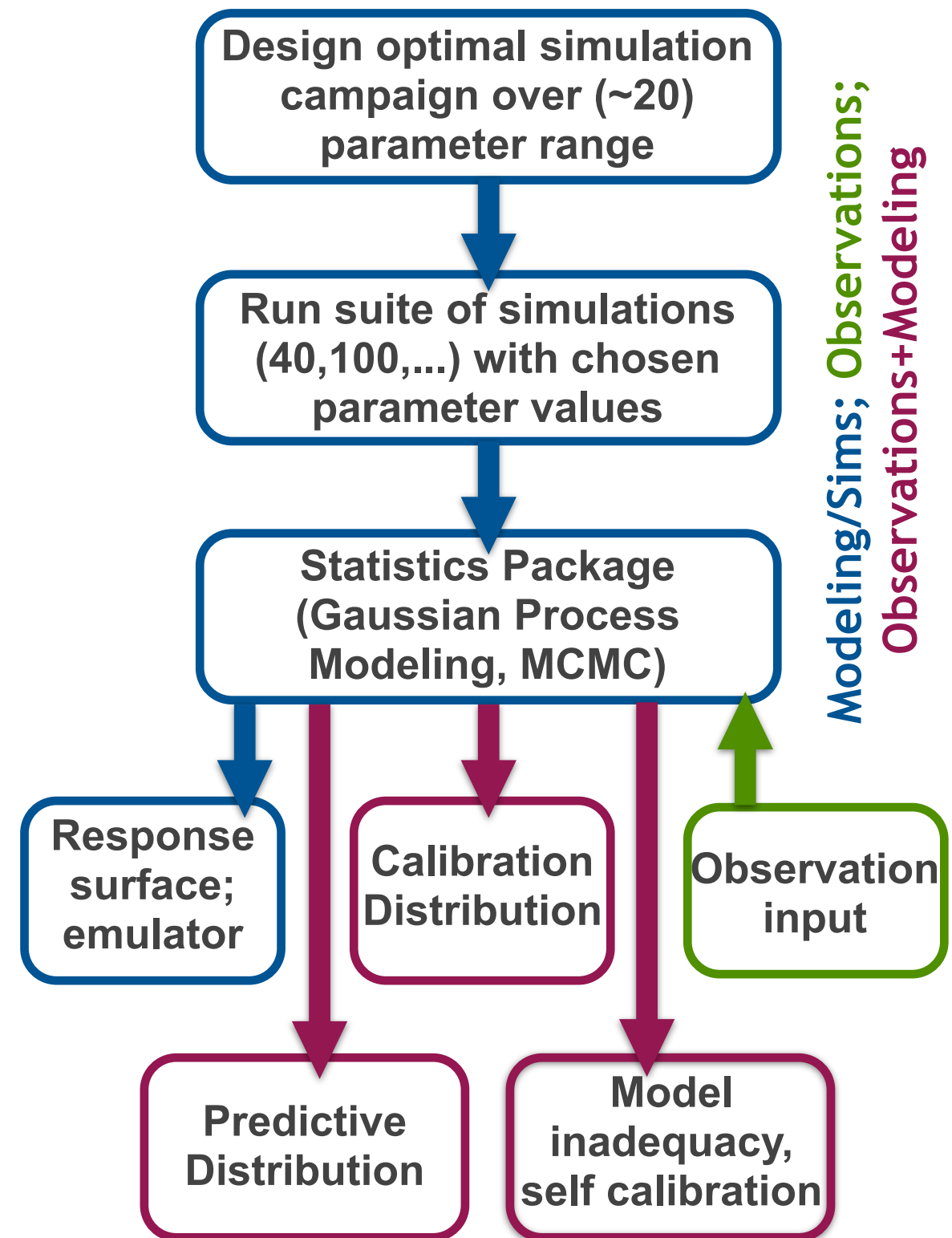


# Solving the Inverse Problem

- **Challenge:** To extract cosmological constraints from observations in non-linear regime, need to run Marko Chain Monte Carlo code; input: 10,000 - 100,000 different models
- **Current strategy:** Fitting functions for e.g.  $P(k)$ , accurate at 10% level, not good enough!
- **Brute force:** Simulations, ~30 years on 2000 processor cluster...
- **Only alternative:** emulators



Heitmann et al. 2006, Habib et al. 2007



# Cosmic Emulator in Action: LSSFast

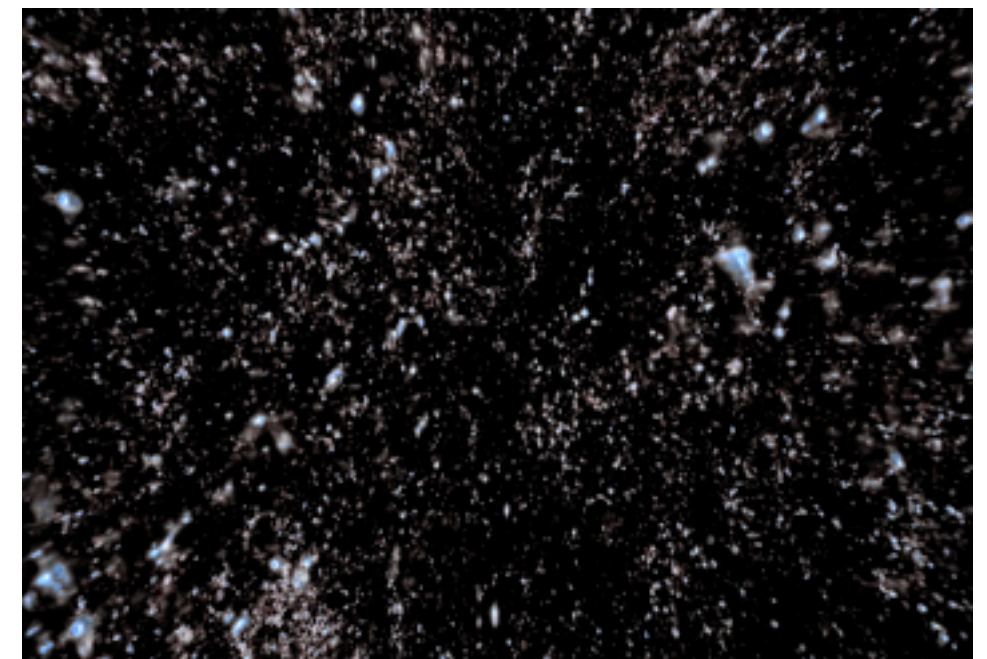
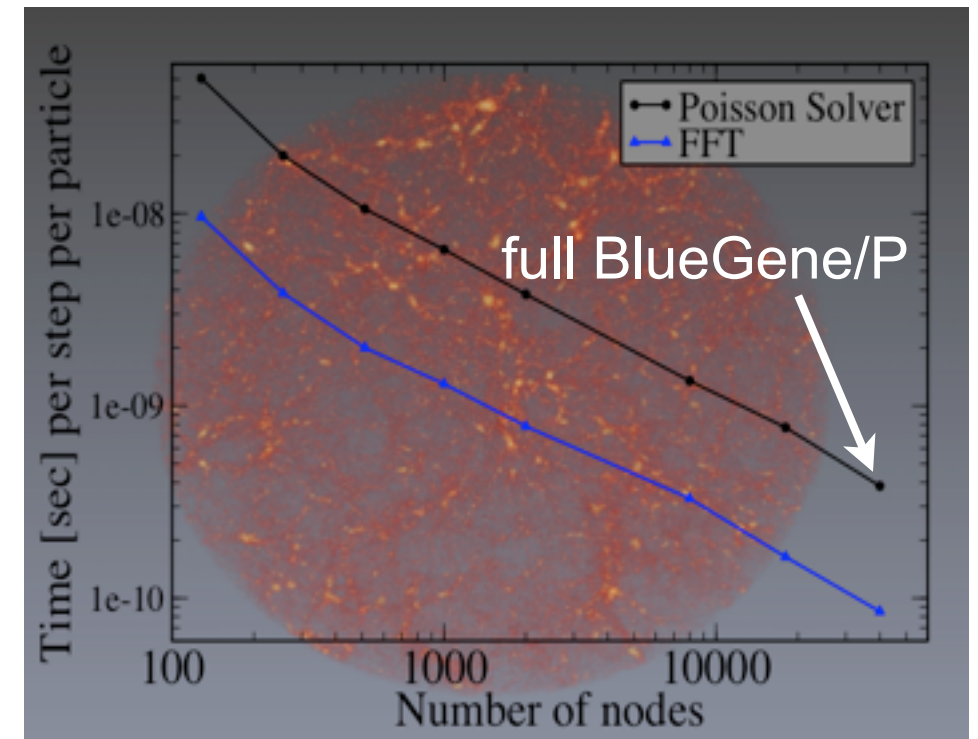
- Instantaneous ‘oracle’ for nonlinear power spectrum, reduces compute time from weeks to negligible, accurate at 1% out to  $k \sim 1/\text{Mpc}$  for  $w\text{CDM}$  cosmologies
- Enables direct MCMC with results from full simulations for the first time





# Hybrid Simulation Codes: HACC and TreePM

- **Hardware Accelerated Cosmology Code (HACC)** (Habib et al. 2009, Pope et al. 2010)
  - New cosmology code designed with major aim of easy portability between different high-performance computing architectures
  - Long-range force: particle mesh, short-range force: particle-particle or tree, architecture dependent
  - Strong collaboration between Los Alamos and Argonne National Labs in code development
  - First version ran on Roadrunner, Cell-accelerated machine, second version on GPU cluster (OpenCL implementation); at SC10: run on heterogenous system with in-situ visualization, now: port to BlueGene system
  - First science: BAO in the Lyman-alpha forest (9 PM runs, 64 billion particles each), precision cosmology with high-resolution code (16 billion particles and up)
- **TreePM** (White 2002)
  - Well established N-body code, used for very large number of science projects: weak lensing, galaxy clustering, BAO, mock catalogs, ...

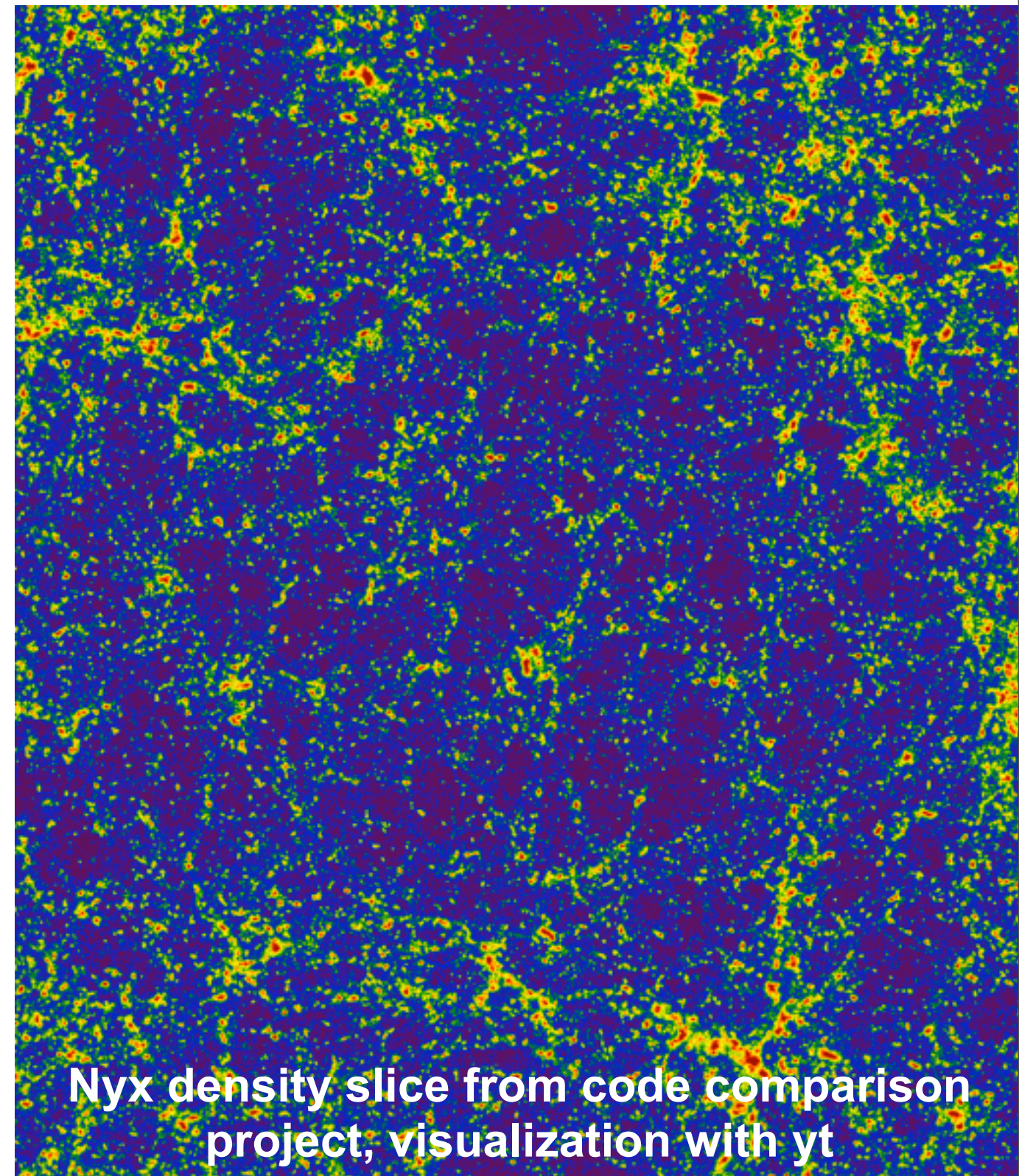


Halos from Roadrunner simulation, visualization: J. Woodring



# Adaptive Mesh Simulation Codes

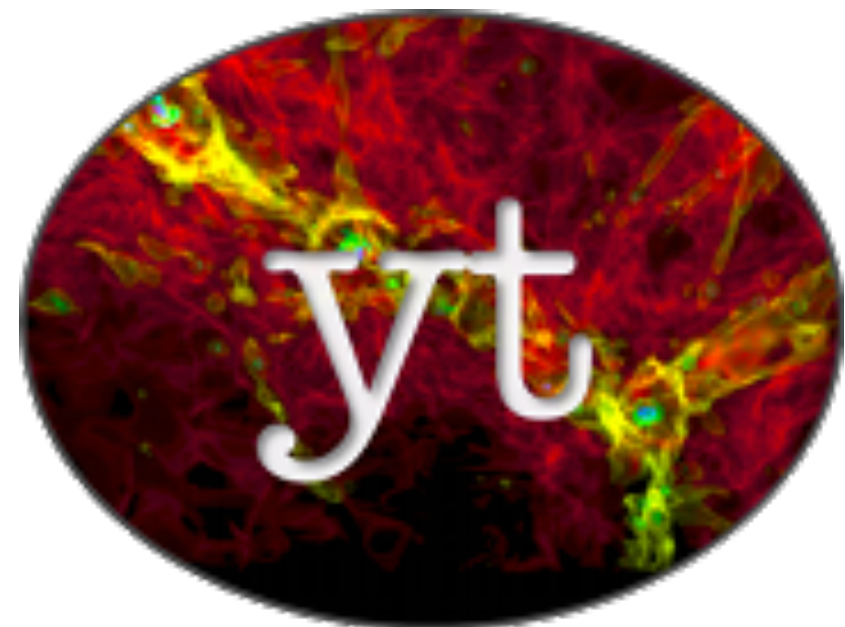
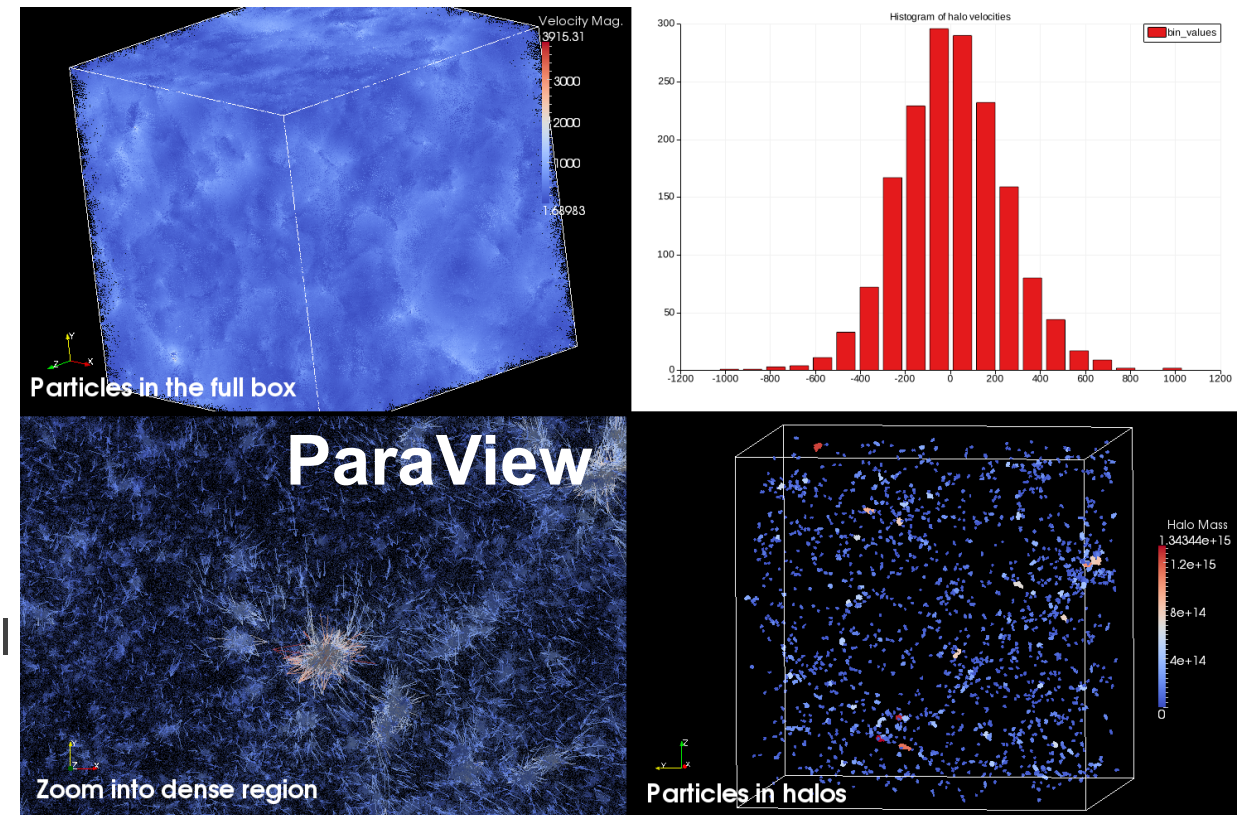
- **Nyx:** New adaptive mesh refinement (AMR) code developed at LBNL
- **Block-structured AMR** with multigrid Poisson solver
- **Main focus for AMR codes** (also Enzo, ART): hydrodynamics simulations, discussed in detail in Nick's talk





# Analysis Capabilities: ParaView and yt

- Analysis of simulations as demanding as carrying out the simulations
- Visualization-aided analysis
  - Visualization is important for understanding the results, and for verification & validation
  - Visualization and analysis have to go hand-in-hand to ensure efficiency
- ParaView (open source)
  - Based on VTK (Visualization Tool Kit), cosmological analysis capabilities focusing on particle data have been developed (LANL/ANL collaboration, J. Ahrens, J. Woodring, P. Fasel, K. Heitmann, S. Habib, J. Insley...)
  - Parallel reader, halo finder, sub-sampler, embedded plotting and analysis routines
- yt (open source)
  - Focus on astrophysical data, AMR, particles also supported, started by Enzo community (SLAC), expanding fast
  - Parallel halo finder, merger trees, ...
  - Lives also within ParaView now



# Some Recent Science Highlights

- Collaboration members have very successful track record in using N-body simulations to explore new physics and analyze survey data
- Cross-laboratory collaborations are established, more being planned
- World-leading capabilities exist

- **Galaxy Surveys**

- The clustering of massive galaxies at  $z \sim 0.5$  from the first semester of BOSS data, M. White et al. ApJ 728, 126 (2011), [LBNL](#)
- Cosmological constraints from galaxy clustering and the the mass-to-number ratio of galaxy clusters, J. Tinker, E. Sheldon, R. Wechsler et al., ApJ (2011), [BNL/SLAC](#)
- Statistics of satellite galaxies around Milky Way-like hosts, M. Busha, R. Wechsler et al, ApJ (2011), [SLAC](#)
- The real-space clustering of luminous red galaxies around  $z < 0.6$  quasars in the Sloan Digital Sky Survey, N. Padmanabhan, M. White, et al., MNRAS 397, 1862 (2009), [LBNL](#)

- **Weak Lensing**

- Probing cosmology with weak lensing peak counts, J. Kratochvil, Z. Haiman, M. May, Phys. Rev. D81, 043519 (2010), [BNL](#)
- Cosmological information in weak lensing peaks, X. Yang, J. Kratochvil, S. Wang, E. A. Lim, Z. Haiman, M. May, Phys. Rev. D84, 043529 (2011), [BNL](#)



# Some Recent Science Highlights

- **Baryon Acoustic Oscillations**
  - **Constraining anisotropic baryon oscillations**, N. Padmanabhan, M. White, Phys. Rev. D77, 123540 (2008), [LBNL](#)
  - **Non-linear structure formation and the acoustic scale**, H.-J.Seo, E.Siegal, D.Eisenstein, M.White, ApJ 686, 13 (2008), [LBNL](#)
  - **Calibrating the baryon oscillation ruler for matter and halos**, N. Padmanabhan, M. White, Phys. Rev. D80, 063508 (2009), [LBNL](#)
- **Baryon Acoustic Oscillations in the Lyman alpha Forest**
  - **The acoustic peak in the Lyman alpha forest**, A. Slosar, S. Ho, M. White, T. Louis, JCAP 10, 019 (2009), [BNL/LBNL](#)
  - **Particle mesh simulations of the Lyman-alpha forest and the signature of baryon acoustic oscillations in the intergalactic medium**, M. White, A. Pope, J. Carlson, K. Heitmann, S. Habib, P. Fasel, D. Daniel, Z. Lukic, ApJ 713, 383 (2010), [LBNL/ANL](#)
- **Redshift Space**
  - **Testing cosmological structure formation using redshift-space distortions**, W. Percival, M. White, MNRAS 393, 297 (2009), [LBNL](#)
  - **Towards an accurate model of the redshift space clustering of halos in the quasilinear regime**, B. Reid, M. White, MNRAS, in press, [LBNL](#)

# Some Recent Science Highlights

- **Clusters and Groups**

- **Mass function predictions beyond LCDM**, S. Bhattacharya, K. Heitmann, M. White, Z. Lukic, C. Wagner, S. Habib, ApJ 732, 122 (2011), [ANL/LBNL](#)
- **Cosmological constraints from the SDSS maxBCG cluster catalog**, E. Rozo, R. Wechsler et al. ApJ, 708, 645 (2010), [SLAC](#)
- **The structure of halos: Implications for group and cluster cosmology**, Z. Lukic, D. Reed, S. Habib, K. Heitmann, ApJ 692, 217 (2009), [ANL](#)

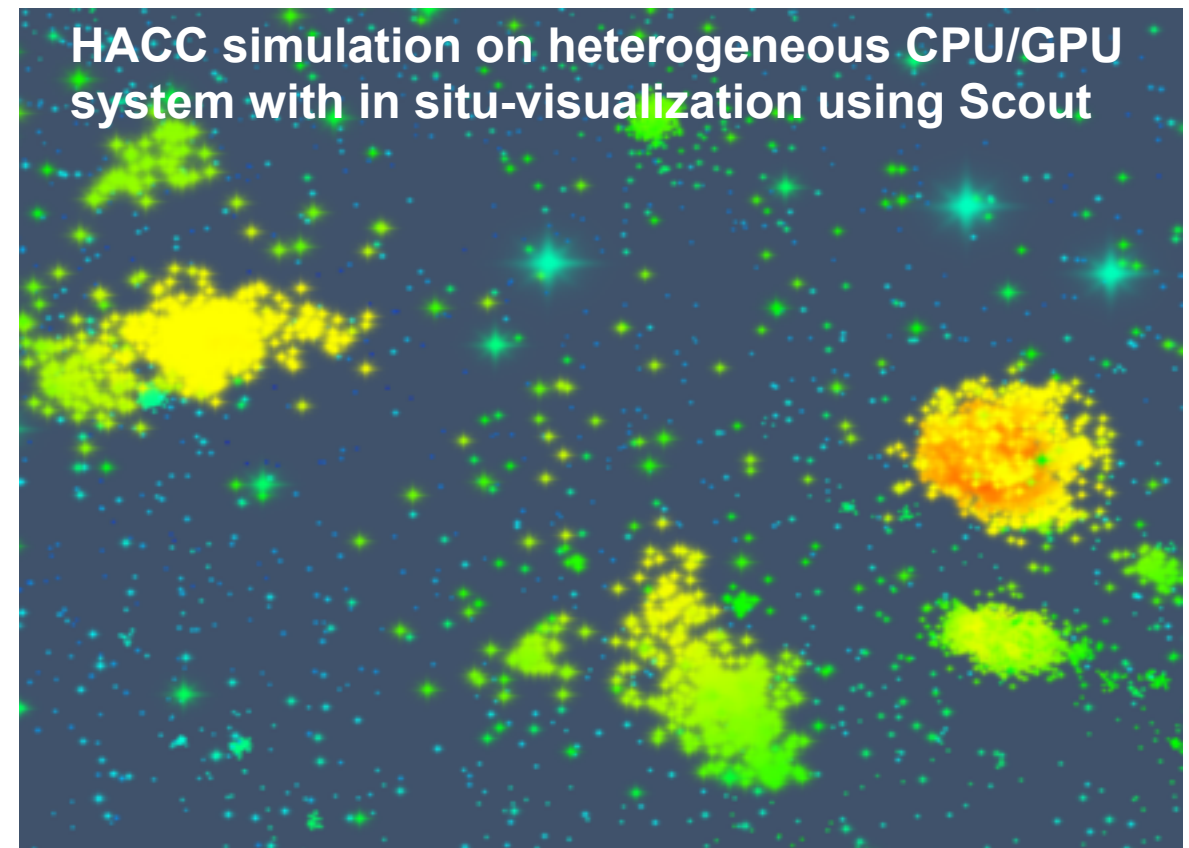
- **Theory**

- **The Coyote Universe III: Simulation suite and precision emulator for the nonlinear matter power spectrum**, E. Lawrence, K. Heitmann, M. White, D. Higdon, C. Wagner, S. Habib, B. Williams, ApJ 713, 1322 (2010), [ANL/LBNL](#)
- **The Coyote Universe I: Precision determination of the nonlinear matter power spectrum**, K. Heitmann, M. White, C. Wagner, S. Habib, D. Higdon, ApJ 713, 1322 (2010), [ANL/LBNL](#)
- **The Cosmic Code Coparison Project**, K. Heitmann, Z. Lukic, P. Fasel, S. Habib, M. Warren, M. White, J. Ahrens, L. Ankeny, R. Armstrong, B. O'Shea, P. Ricker, V. Springel, J. Stadel, H. Trac, Compt. Sci. Dis. 1, 015003 (2008), [ANL/LBNL](#)

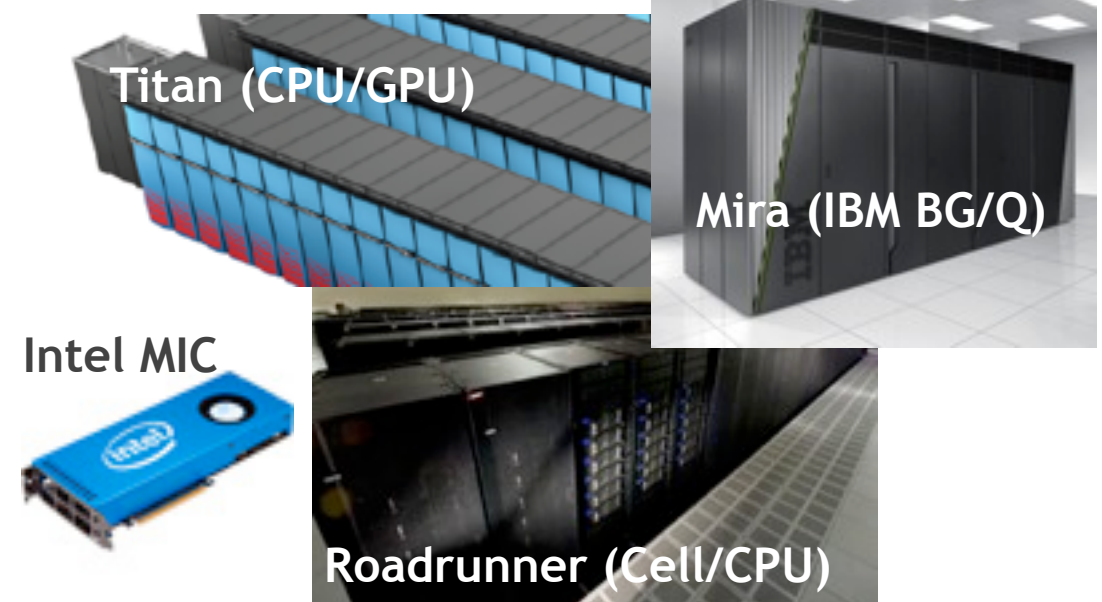


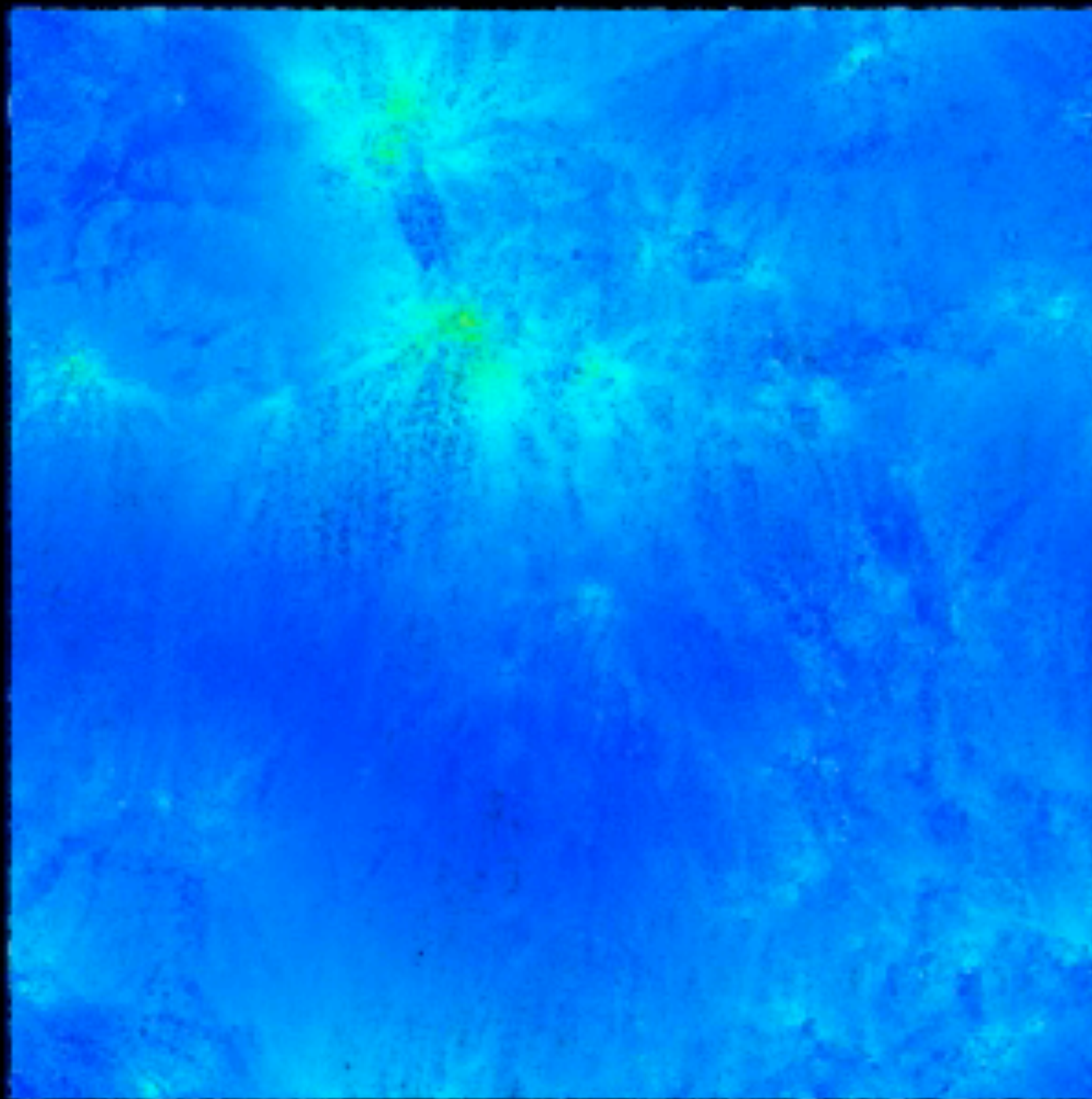
# Challenges for the Future

- Large cosmological volumes with  $\sim$  trillion particles are needed for ongoing and future large scale surveys
  - Hundreds to thousands of realizations, not only for one cosmology!
  - Coverage of cosmological model space
  - Error control in simulations
  - Supercomputer architectures are changing! Codes need to be flexible, **close collaboration with computer science community very beneficial**
  - Simulation analysis, **close collaboration with CS community very beneficial**
  - Data serving, **close collaboration with CS community very beneficial**
- Outstanding opportunity for HEP and ASCR to work close together and make an impact!
  - National Laboratories poised to carry out an effort that can benefit the community

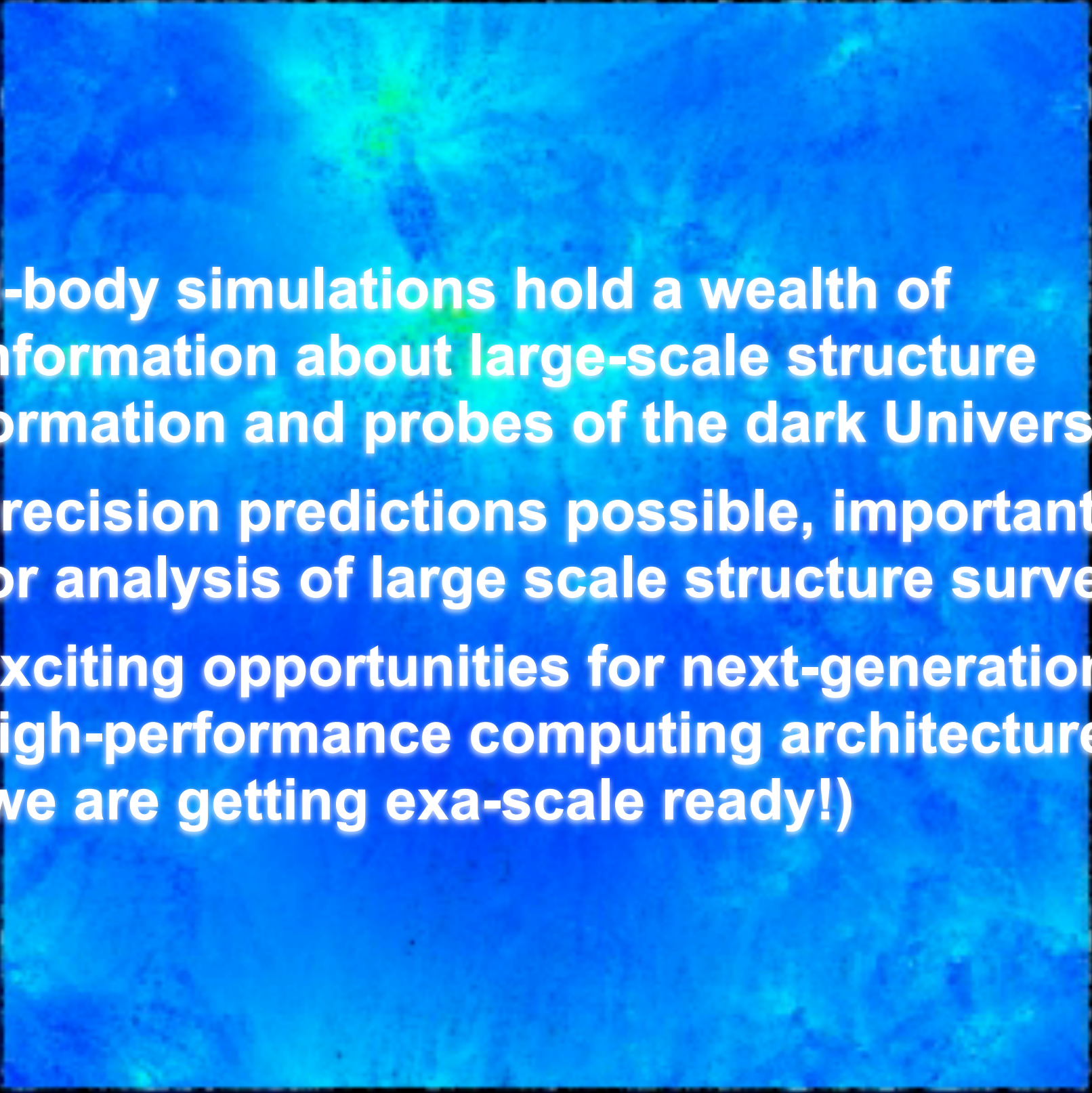


## “Architecture Zoo”







- 
- **N-body simulations hold a wealth of information about large-scale structure formation and probes of the dark Universe**
  - **Precision predictions possible, important for analysis of large scale structure surveys**
  - **Exciting opportunities for next-generation high-performance computing architectures (we are getting exa-scale ready!)**